

## A CHEMICAL STUDY OF *Lagochilus pubescens*

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The genus *Lagochilus*, family Labiatae, is represented in Central Asia by approximately 30 species [1]. Lagochiline and lagochiline tetraacetate have been isolated from individual species [2, 3], and a number of flavonoids have also been identified chromatographically [4, 5].

We have investigated *Lagochilus pubescens* collected in the village of Ak-Tuprak, Kirghiz SSR (1972). The comminuted air-dry raw material (3.9 kg) was extracted with acetone (80 liters). The acetone extracts were concentrated to small volume and diluted with water and were then extracted successively with petroleum ether, hexane, benzene, diethyl ether, and chloroform.

The petroleum-ether extract was evaporated to dryness, and the residue (29 g) was chromatographed on a column of silica gel. Elution was performed with a mixture of diethyl ether and petroleum ether (2:1). Four individual substances were isolated.

Substance (I), composition  $C_{29}H_{60}$ , mp 63°C (from petroleum ether) corresponded in its physicochemical constants to nonacosane [6].

Substance (II), with the composition  $C_{17}H_{15}O_5$ , mp 173-174°C (from acetone),  $M^+$  298,  $R_f$  0.80 [chloroform-acetone (9:1)], formed a monoacetyl derivative with a melting point of 196-197°C (from ethanol). Its UV spectrum had maxima at 210, 266, and 326 nm and its IR spectrum absorption bands at 1620, 1520, and 1455  $cm^{-1}$  (carbonyl of a 5-hydroxy- $\gamma$ -benzopyrone), 1600  $cm^{-1}$  (aromatic nucleus), and 2970-3120  $cm^{-1}$  ( $-OCH_3$ ).

On the basis of qualitative reactions and the characteristics of its UV, IR, and mass spectra it was established that the substance is 5-hydroxy-4',7-dimethoxyflavone [7], and this was confirmed by its PMR spectrum. The PMR spectrum, taken in acetone (Varian XL-100,  $\delta$  scale, HMDS), showed a six-proton singlet at 3.82 ppm ( $2-OCH_3$ ), doublets at 6.2 and 6.54 ppm due to  $C_6$  and  $C_8$  protons, a singlet at 6.56 ppm corresponding to a proton at  $C_2$  of the pyrone ring, doublets at 7.00 and 7.9 ppm corresponding to protons at  $C_{3',5'}$  and  $C_{2',6'}$ ; the proton of a hydroxy group at  $C_5$  was observed in the 12.78 ppm region.

Substance (III), with the composition  $C_{29}H_{50}O$ , mp 137-138°C (from methanol) corresponded in its spectral characteristics to  $\beta$ -sitosterol, as was confirmed by a direct comparison with an authentic sample of  $\beta$ -sitosterol.

Substance (IV), with the composition  $C_{20}H_{36}O_5$ , mp 167-168°C (from acetone), had  $[\alpha]_D^{25} -9.13^\circ$  (c 3, ethanol). From its IR, mass, and PMR spectra it corresponded to lagochiline. However, according to the literature [8], lagochiline has a somewhat lower melting point (157-158°C) and is optically inactive.

This is the first time that nonacosane, 5-hydroxy-4',7-dimethoxyflavone, and  $\beta$ -sitosterol have been found in the genus *Lagochilus*.

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